Message

Sent: 8/29/2019 11:17:51 AM
To: Volz, Stephanie [/o=ExchangeLabs/ou=Exchange Administrative Group (FYDIBOHF23SPDLT)/cn=Recipients/cn=56abdbfdc7cc496ea71c6ac9ce20c36c-SVOLZ]
CC: Leung, Lam-Wing H [LAM.H.LEUNG-1@chemours.com]
Subject: RE: PFAS Question

Stephanie,

Are your samples from the Chemours facility in the Fayetteville, NC area? If so I would expect some of the PFO5DoDa.

The n-methyl FOSE and n-ethyl FOSE are alcohols and are not anionic so they will come out in the methanol wash of the WAX cartridge for sure. If the FTOHs were present they would as well. Also the PFOSA (or any other sulfonamide) washes out at this step. We found we lost that one in the EPA 24 mix first time we tried it.

I have been looking for ADONA in samples I get but have yet to see it. If I were near a 3M facility I think I would see some.

With respect to the PFAS standards you list below, I have all of them. However, they are quite dated and I got them all from Chemours disolved in water. I do think these would be fine for compound confirmation but not for quantitation. I am glad to send you some of mine, however it is possible you could get fresh stocks from Chemours for you if you ask. My contact there is Lam Leung LAM.H.LEUNG-1@chemours.com

I do have PFMOAA solid and I have some PFESA BP2 disolved in methanol at a high concentration but not solid. PFESA BP2 is now available from Synquest Labs http://www.synquestlabs.com/product/id/143103.html

PFMOAA is available from Synquest Labs http://www.synquestlabs.com/product/id/143107.html

Or from Fluoryx

From: Volz, Stephanie <Volz.Stephanie@epa.gov>
Sent: Wednesday, August 28, 2019 4:48 PM
To: Strynar, Mark <Strynar.Mark@epa.gov>
Subject: RE: PFAS Question

Excellent. Thank you so much. It appears I have PFO5DoDA in my samples.

We would love to get our hands on some reference material. How can I make that happen? We're analyzing water samples for these compounds and I'm sure you know what other compounds are up and coming on the horizon (ADONA...).

Perfluoro-3,6-dioxa-4-methyl-7-octene-1-sulfonic acid	PFESA Byproduct 1*	29311-67-9	$C_7HF_{13}O_5S$	443.93371
2-[1-[difluoro(1,2,2,2-tetrafluoroethoxy)methyl]-1,2,2,2-	PFESA Byproduct 2*	749836-20-2	$C_7H_2F_{14}O_5S$	463.93994

tetrafluorooexthoxy]-1,1,2,2-tetrafluoro-ethanesulfonic acid				
2,2-difluoro-2-(trifluoromethoxy) acetic acid	PFMOAA*	674-13-5	$C_3HF_5O_3$	179.98459
Perfluoro-3,5-dioxahexanoic acid	PFO2HxA*	39492-88-1	$C_4HF_7O_4$	245.97631
Perfluoro-3,5,7-trioxaoctanoic acid	PFO3OA*	39492-89-2	$C_5HF_9O_5$	311.96803
Perfluoro-3,5,7,9-tetraoxadecanoic acid	PFO4OA*	39492-90-5	$C_6HF_{11}O_6$	377.95975
Perfluoro-3,5,7,9, 11-pentadoddecanoic acid	PFO5OA or TAFN4*	39492-91-6	$C_7HF_{13}O_7$	443.95147
Propanoic Acid, 2,2,3,3-tetrafluoro-3-(trifluoromethoxy)-	PFECA F or PMPA*	377-73-1	$C_4HF_7O_3$	229.98139

We were also trying to quantify N-MeFOSE and N-EtFOSE but were unable to recover the associated internal standards. We did additional washes of the SPE cartridge and now we're thinking they may have washed through during the column conditioning. We still need to test that theory out.

Thanks again,
Steph

From: Strynar, Mark <Strynar.Mark@epa.gov>
Sent: Wednesday, August 28, 2019 2:02 PM
To: Volz, Stephanie <Volz.Stephanie@epa.gov>
Subject: RE: PFAS Question

Stephanie,

First for the PFESA BP2, yes having two peaks is typical. Something about having asymmetric carbons or something like that. I don't recall the details. The peaks are usually exactly the same size, but for sure 2 peaks.

For the PFESA BP1 and the PFO5DoDA they are similar in molecular weight however two things will stand out.

1. The molecular weight between two compounds PFESA BP1 (442.9264) and PFO5DoDA (442.9442) is 40.2 ppm. Your QTOF should be able to tell them apart based on mass due to the EIC being extracted can be chosen to be +/- 5 ppm or so.
2. The PFESA BP1 will have a sulfonate (m/z 79.9) and a FSO3 (m/z 98.9) transition just like the PFOS, PFHxS and PFBS do.

3. PFO5DoDA will have a 84.9907 fragment however the PFESA BP1 will not. I have no idea what the 283.1367 fragment is. Also it will

Glad to chat if you need more later on tomorrow. Here is my 2015 paper in the SI that may have some details you can use. I also have standards for all of these I can share if you need them.

Mark

From: Volz, Stephanie <Volz.Stephanie@epa.gov>
Sent: Wednesday, August 28, 2019 3:06 PM
To: Strynar, Mark <Strynar.Mark@epa.gov>
Subject: PFAS Question

Mark,
I just left you a phone message but was wondering if you have any insight or documentation into telling these two compounds (PFESA Byproduct 1 and PFO5DA) apart. I don't have any reference material but I am working on a QTOF. I'm seeing 442.943 and 886.896 for the dimer. I'm seeing the peak at 8.175 minutes and fragments of 283.1367 and 84.9907. I don't have background data on retention time or fragments for either compound.

Compound Name	Formula	RT (min)	Mass	m/z	Adduct/dimer	Fragments	Fragments	Fragments	CAS	IUPAC N
PFESA (Byproduct 1)	C7HF13O5S		443.93371	442.9441926	886.8596 (2M-H)-	?	?	?	29311-67-9	Perfluoro-3,
PFO5DA	C7HF13O7		443.95147	442.926434	886.8951 (2M-H)-	?	?	?	39492-91-6	Perfluro-3,5

Also, I'm seeing a doublet for PFESA Byproduct 2 at 7.171 and 7.294 minutes. Do you know if that's typical?

Best Regards,

Stephanie Volz
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